

A Fast Approach to Creative Telescoping

Christoph Koutschan

Abstract. In this note we reinvestigate the task of computing creative telescoping relations in differential-difference operator algebras. Our approach is based on an ansatz that explicitly includes the denominators of the delta parts. We contribute several ideas of how to make an implementation of this approach reasonably fast and provide such an implementation. A selection of examples shows that it can be superior to existing methods by a large factor.

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1. Introduction

The method of creative telescoping nowadays is one of the central tools in computer algebra for attacking definite integration and summation problems. Zeilberger with his celebrated holonomic systems approach [17] was the first to recognize its potential for making these tasks algorithmic for a large class of functions. In the realm of holonomic functions, several algorithms for computing creative telescoping relations have been developed in the past. The methodology described here is not an algorithm in the strict sense because it involves some heuristics. But since it works pretty well on nontrivial examples we found it worth to be written down. Additionally we believe that it is the method of choice for really big examples. Our implementation is contained in the Mathematica package `HolonomicFunctions` as the command `FindCreativeTelescoping`. The package can be downloaded from the RISC combinatorics software webpage:

<http://www.risc.uni-linz.ac.at/research/combinat/software/>

Throughout this paper we will work in the following setting. We assume that a function f to be integrated or summed satisfies some linear difference-differential relations which we represent in a suitable operator algebra (Ore algebra). We use the symbol D_x to denote the derivation operator w.r.t. x and S_n for the shift operator w.r.t. n . Such an algebra can be viewed as a polynomial ring in the respective operators, with coefficients being rational functions in the corresponding variables, subject to the commutation rules $D_x x = x D_x + 1$ and $S_n n = n S_n + S_n$. Ideally, all the relations for f generate a ∂ -finite left ideal, i.e., a zero-dimensional left ideal in the operator algebra. If additionally f is holonomic (a notion that can be made formal by D -module theory), then the existence of creative telescoping relations is guaranteed by theory (i.e., by the elimination property of holonomic modules). Chyzak, Kauers, and Salvy [6] have shown that creative telescoping is also possible for higher-dimensional ideals under certain conditions. We tacitly assume that any input to a creative

telescoping algorithm is ∂ -finite and holonomic, and that it is given as a left Gröbner basis G of the annihilating ideal of f .

The main concern of this paper is to compute creative telescoping relations for an integrand (resp. summand) $f(v, \mathbf{w})$ where v is the integration (resp. summation) variable and $\mathbf{w} = w_1, w_2, \dots$ are some additional parameters. In other words, we are looking for annihilating operators for $f(v, \mathbf{w})$ of the form

$$P(\mathbf{w}, \partial_{\mathbf{w}}) + \tilde{\partial}_v \cdot Q(v, \partial_v, \mathbf{w}, \partial_{\mathbf{w}}) \quad (1.1)$$

where ∂_v and $\tilde{\partial}_v$ stand for operators acting on the variable v ($\partial_v = \tilde{\partial}_v = D_v$ in the case of an integral, and $\partial_v = S_v$ and $\tilde{\partial}_v = S_v - 1$ in the summation case), and $\partial_{\mathbf{w}}$ are the operators $\partial_{w_1}, \partial_{w_2}, \dots$ that correspond to the extra parameters. We will refer to P as the principal part (also known as the telescoper), and to Q as the delta part. From (1.1) it is immediate to derive relations for the definite integral (resp. sum), which in general can be inhomogeneous. Similarly, multiple integrals and sums can be done by creative telescoping relations that correspond to an operator of the form

$$P(\mathbf{w}, \partial_{\mathbf{w}}) + \tilde{\partial}_{v_1} \cdot Q_1(\mathbf{v}, \mathbf{w}, \partial_{\mathbf{v}}, \partial_{\mathbf{w}}) + \tilde{\partial}_{v_2} \cdot Q_2(\mathbf{v}, \mathbf{w}, \partial_{\mathbf{v}}, \partial_{\mathbf{w}}) + \dots \quad (1.2)$$

where $\mathbf{v} = v_1, v_2, \dots$ denote the integration (resp. summation) variables (also mixed cases are possible); we will use the notation $\mathbf{v}^\alpha = v_1^{\alpha_1} v_2^{\alpha_2} \dots$. Note that in general the application of (1.2) yields a relation with inhomogeneous right-hand side that consists of integrals (resp. sums) of one dimension lower. These can be treated recursively in the same way.

2. Description of the method

The known algorithms for computing creative telescoping relations for holonomic functions are either based on elimination (e.g., by rewrite rules / Gröbner bases) or on the use of an ansatz with undetermined coefficients. Zeilberger's slow algorithm [17] and Takayama's algorithm [14, 13, 7] fall into the first category. Their advantage is that they can deal with multiple integrals and sums, but elimination can be a very difficult task and moreover, it is not guaranteed that they deliver the smallest relations that exist in the given annihilating ideal. A relatively small (and hypergeometric!) example that so far has resisted the elimination approach is given in Section 3.3. Since the algorithms that we are going to discuss here fall into the second category, we do not want to go into further detail with elimination-based algorithms.

All the other algorithms make an ansatz with undetermined coefficients. Reduction modulo the Gröbner basis G gives its normal form representation. For the creative telescoping relation to be in the ideal generated by G , its normal form must be identically zero. Hence equating all coefficients of the normal form to zero gives rise to a system of equations that can be solved for the undetermined coefficients. The algorithms described below differ only in the shape of the ansatz.

A classical algorithm that is based on an ansatz has been proposed by Chyzak [5]. It can only be applied to single integrals or single sums, and has to be used in an iterative way for multiple ones. With the notation of (1.1) its ansatz is of the following form:

$$\sum_{\beta \in B} p_\beta(\mathbf{w}) \partial_{\mathbf{w}}^\beta + \tilde{\partial}_v \cdot \sum_{\gamma \in U} q_\gamma(v, \mathbf{w}) (\partial_v, \partial_{\mathbf{w}})^\gamma \quad (2.1)$$

where B is a finite multi-index set and U is the finite set of multi-indices that correspond to the monomials under the stairs of the Gröbner basis G . The unknown $p_\beta(\mathbf{w})$ are rational functions in $\mathbb{K}(\mathbf{w})$, and the unknown $q_\gamma(v, \mathbf{w})$ are rational functions in $\mathbb{K}(v, \mathbf{w})$. When the ansatz (2.1) is written in standard operator representation, i.e., when $\tilde{\partial}_v$ is commuted to the right, we encounter derivatives (resp. shifts) of the $q_\gamma(v, \mathbf{w})$ with respect to v . Finally, we end up with a coupled linear

first-order system of differential (resp. difference) equations. All implementations of Chyzak's algorithm that we know of¹ uncouple this system and then solve the resulting scalar equations one by one. Experience shows that these steps can be extremely costly, in particular when U is big. As an alternative to uncoupling there are algorithms for directly solving such coupled systems, proposed by Abramov and Barkatou [1, 4]. A comparison of how these methods perform on big creative telescoping examples could be an interesting research topic for the future. However, in this article we want to follow a different way of bypassing the bottleneck, namely by means of a different ansatz that does not lead to a coupled system.

In [10, 11] a first step into this direction has been taken by means of a “polynomial ansatz” of the form

$$\sum_{\beta \in B} p_{\beta}(\mathbf{w}) \partial_{\mathbf{w}}^{\beta} + \tilde{\partial}_{v_1} \cdot \sum_{\gamma \in C_1} \sum_{\alpha \in A_1} q_{1,\alpha,\gamma}(\mathbf{w}) v^{\alpha} (\partial_v, \partial_w)^{\gamma} + \dots \quad (2.2)$$

where A_i , B , and C_i are finite sets of multi-indices, and the dots hide terms with $\tilde{\partial}_{v_2}, \dots$. The unknown p_{β} and $q_{i,\alpha,\gamma}$ to solve for are rational functions in the surviving variables \mathbf{w} and they can be computed using pure linear algebra, without any uncoupling needed (since commuting the $\tilde{\partial}_{v_i}$ to the right will not affect them). Note also that the summation variables will not occur in the denominators. The price that we pay is that the shape of the ansatz is not at all clear from the beginning: The sets A_i , B , and C_i need to be fixed, whereas in Chyzak's algorithm we have to loop only over the support of the principal part (the set B). Another drawback of this ansatz is the fact that the delta parts in this denominator-free representation usually have not only much bigger supports ($|C_i| > |U|$), but also higher polynomial degrees and larger integer coefficients than the reduced representation returned by Chyzak's algorithm². Of course, once found, the solution of the polynomial ansatz can be transformed to reduced representation yielding the same result as Chyzak's algorithm in the one-dimensional case (just reduce the delta part with the Gröbner basis G). So we have now got rid of the uncoupling problem, but the above observation suggests that the result of the polynomial ansatz is blown up unnecessarily and that we can do even better.

And in fact, we can! The only thing we have to do is to include the denominators of the delta parts into the ansatz:

$$\sum_{\beta \in B} p_{\beta}(\mathbf{w}) \partial_{\mathbf{w}}^{\beta} + \tilde{\partial}_{v_1} \cdot \sum_{\gamma \in U} \sum_{\alpha \in A_1} \frac{q_{1,\alpha,\gamma}(\mathbf{w}) v^{\alpha}}{d_{1,\gamma}(\mathbf{v}, \mathbf{w})} (\partial_v, \partial_w)^{\gamma} + \dots \quad (2.3)$$

where the notation is as in (2.2) except that we can restrict the support of the delta part to the monomials under the stairs of G (as in Chyzak's algorithm). The denominators $d_{i,\gamma}$ are polynomials in $\mathbb{K}[\mathbf{v}, \mathbf{w}]$. After coefficient comparison with respect to \mathbf{v} we finally have to solve a linear system in the p_{β} and the $q_{i,\alpha,\gamma}$ over $\mathbb{K}(\mathbf{w})$. This means that when we will be talking about the denominators $d_{i,\gamma}$, we will refer solely to those parts (factors) of the $d_{i,\gamma}$ that actually involve some of the variables \mathbf{v} ; the remaining factors will be contributed from the solutions $q_{i,\alpha,\gamma}$ over $\mathbb{K}(\mathbf{w})$.

Now it is no secret that the denominators $d_{i,\gamma}$ can be somehow predicted: We do not know them a priori, but we can deduce a list of candidate factors that might appear within them. In the hypergeometric case, Wilf and Zeilberger [16] already have described how to get a good guess on the denominators. In general it is not difficult to see that the leading coefficients of the Gröbner basis G play the key rôle: consider a solution of the form (2.2) (that is guaranteed to exist by the elimination property, provided that f is holonomic) and reduce its delta part with G to obtain a representation of the form (2.3). It is now clear that a solution must exist where only factors from the leading coefficients of G as well as their shifted instances appear in the denominators.

¹Besides our Mathematica package `HolonomicFunctions`, this refers to Chyzak's implementation which is part of the Maple package `MgfFun` (<http://algo.inria.fr/libraries/>).

²To give some quantitative results: in the TSPP example, see Section 4, we ended up with polynomial degrees up to 764 and integer coefficients with up to 378 digits, whereas the reduced representation has degree 120 and at most 74-digit integers.

The rest of this section will be dedicated to explaining how this technique can be completely automatized and made reasonably fast. For example, the implementations of the hypergeometric case that use ansatz (2.3) (by Zeilberger³ in Maple, and by Wegschaider⁴ in Mathematica) require the denominators explicitly as input. Moreover, Wegschaider in his thesis [15] states that ansatz (2.2) is preferable to (2.3) even when the denominators are known. We do not share his opinion, as we shall demonstrate below. Or more concretely, we do not think that this statement holds in the general (not necessarily hypergeometric) case.

In all ansatz-based algorithms (and hence in our approach), the main loop is over the support of the principal part. In the following we concentrate on one single step, i.e., we assume that the set B is fixed, and describe our implementation by explaining the various optimizations that we have included.

Optimization 1. To get started with, we need some heuristics for guessing the denominators $d_{i,\gamma}$. It seems to be natural to start with a common denominator d , i.e., $d_{i,\gamma} \mid d$ for all i and all γ . Ideally, a good heuristic should always deliver a d that is indeed a multiple of all the denominators, but without overshooting too much. Experiments suggest that it suffices to take the denominators that occur during the reduction of the whole ansatz; recall that its support is already fixed which allows for a very fast “simulated reduction” where we do not compute with coefficients but only with supports.

Optimization 2. Once we have a good candidate for the common denominator we have to test whether for this setting, i.e., for the principal part under consideration, there exists a solution. Additionally we still have to fix the degrees of the ansatz (the sets A_i); see the next step for this issue. To see whether there is a solution we have to reduce the ansatz with the Gröbner basis G and solve the corresponding linear system. And of course, it suffices to perform these steps in a homomorphic image. Hence we plug in some concrete integers for the parameters w and reduce all integer coefficients modulo a prime⁵. If there is no solution in the homomorphic setting, there is, a fortiori, no solution in the general setting. By choosing these values sufficiently generically we can also minimize the risk of obtaining a homomorphic solution that does not extend to a general solution. There is one important point to mention and this concerns the reduction modulo G : we are working in a noncommutative algebra and therefore it is problematic to replace an indeterminate by an integer, since by doing so, we loose the noncommutativity between this indeterminate and the operator that is connected to it. In [11] we have described a modular reduction procedure that keeps track of this issue. The basic idea is that in each step of the reduction process we have to do the noncommutative multiplication of a Gröbner basis element that makes the leading power products match, in the general setting, but everything else in the homomorphic setting since no noncommutativity is involved any more.

Optimization 3. We still do not know which v -degrees in the numerators of our ansatz we should try. It is manifest to start with small degrees and increase them until either the homomorphic computations indicate that a solution might exist or the degrees become unreasonably large (hence here is a second heuristic involved). The following observation suggests that we can be quite generous with setting an upper bound for the degrees. Let T be the ansatz (2.3) and T' its counterpart with the increased degrees (for this reasoning it is irrelevant whether we talk about the total degree in v or the componentwise degrees; in any case we have some $A'_i \supseteq A_i, i = 1, 2, \dots$). Then the unknowns that appear in $T' - T$ are precisely the $q_{i,\alpha_i,\gamma}$ with $\alpha_i \in A'_i \setminus A_i$. Obviously the sets of undetermined coefficients occurring in T and $T' - T$ have empty intersection. Hence we do not have to build the whole linear system from scratch, but instead in each step of the degree-looping we have to reduce only the new part $T' - T$ and add some columns (and possibly rows) to the matrix. In our

³<http://www.math.rutgers.edu/~zeilberg/programs.html>

⁴<http://www.risc.uni-linz.ac.at/research/combinat/software/MultiSum/>

⁵in our implementation, we choose 7-digit integers for the w and as modulus the largest prime that fits into a machine word, i.e., 2147483629.

implementation we have decided to loop over an integer δ such that δ limits the degree of each of the variables v . Once a homomorphic solution is found for a certain δ we can refine the degree setting componentwise by a few more modular nullspace computations.

Optimization 4. Ok, let's now assume that we found a homomorphic solution for some principal part, some common denominator d and some degree setting A_i . We could now use this ansatz to start the final computation, but there is still lots of possibilities for improvement. Recall that at this point we only have some common multiple of the denominators, but not necessarily the minimal one. Again using homomorphic computations, it is not difficult and not very costly to figure out the least common multiple of all the denominators: for each factor of d we check whether deleting this factor and decreasing the degree setting of the numerators accordingly, still yields a solution. If so, we can remove this factor from our ansatz. Note that such unnecessary factors in the denominator blow up the degrees of the numerator, too, since they have to cancel in the end.

Optimization 5. But should we stop after minimizing the common denominator? In the very same fashion, we can now proceed to minimize each single denominator $d_{i,\gamma}$. Note that for small examples this overhead can consume a considerable part of the total computation time. However, we are definitely convinced that it pays off in big examples.

Optimization 6. Last but not least we omit all undetermined coefficients from our ansatz that are zero in the homomorphic image. They most probably will be zero in the end—but this is folklore...

3. Examples

In this section we want to present some examples that illustrate the applicability of our ansatz. To have a fair comparison of the timings, we do all computations in the same computer algebra system (Mathematica) and we want to mention that all the code has been implemented by the same person (unless stated otherwise). The results are listed in Table 1.

Example	Ansatz (2.1)			Ansatz (2.3)		
	time	memory	output	time	memory	output
Bessel	127	78	7.2	10	1.9	7.2
Gegenbauer	1122	601	13	1.6	0.66	13
Andrews-Paule	27	30	341	2.1	0.35	4.3
Feynman (wz)	81	156	293	174	85	156
Feynman (zw)	171	126	91			

TABLE 1. Timings (in seconds), memory usage (in MegaBytes), and output size (in KiloBytes) for Chyzak's algorithm and our ansatz; the Feynman example consists of two rows corresponding to the different orders of integration (in the double sum, changing the summation order does not lead to different values).

3.1. Integral with four Bessel functions

An example that is often used for testing creative telescoping procedures is the following integral over a product of four Bessel functions

$$\int_0^\infty x J_1(ax) I_1(ax) Y_0(x) K_0(x) dx = -\frac{\log(1-a^4)}{2\pi a^2}. \quad (3.1)$$

The intriguing fact with this example is that the input, the annihilating ideal for the integrand

$$\{a^3 D_a^4 + 4a^2 D_a^3 - 3a D_a^2 + 3D_a + 4a^3 x^4, \\ x^4 D_x^4 - 4ax^3 D_x^3 D_a + 6a^2 x^2 D_x^2 D_a^2 - 4a^3 x D_x D_a^3 + 12ax^2 D_x^2 D_a - 24a^2 x D_x D_a^2 + \\ 8a^3 D_a^3 + x^2 D_x^2 - 26ax D_x D_a + 40a^2 D_a^2 - 3x D_x + 26a D_a - 4a^4 x^4 + 4x^4 + 3\}$$

as well as the output, the creative telescoping operator

$$aD_a + 2 + D_x \cdot \frac{1}{4(a^4 - 1)x^3} \cdot (-ax^3 D_x^3 D_a + 4a^2 x^2 D_x^2 D_a^2 - 6a^3 x D_x D_a^3 - 2x^3 D_x^3 \\ + 12ax^2 D_x^2 D_a - 32a^2 x D_x D_a^2 + 16a^3 D_a^3 - 25ax D_x D_a \\ + 70a^2 D_a^2 - 2x D_x + 19a D_a - 16a^4 x^4 + 2) \quad (3.2)$$

are pretty small. In particular, observe that the principal part is of order 1, and hence no longish looping is necessary. But the integrand, being a product of four Bessel functions (which are ∂ -finite with dimension 2), has an annihilating ideal that contains $16 = 2 \cdot 2 \cdot 2 \cdot 2$ monomials under its stairs, and this causes Chyzak's algorithm to take quite long with finding (3.2) (recall that a 16 by 16 system of differential equations has to be uncoupled which causes intermediate expression swell). Therefore the timings and memory usages differ by more than one order of magnitude: 10s vs. 127s, and 1.9MB vs. 78MB, respectively.

3.2. A product of three Gegenbauer polynomials

The following identity can be found as formula (6.8.10) in the book by Andrews, Askey, and Roy [2]. It is valid when $\lambda > -\frac{1}{2}$ and $\lambda \neq 0$, $l + m + n$ is even and the sum of any two of l, m, n is not less than the third. The integral is zero in all other cases:

$$\int_{-1}^1 C_l^{(\lambda)}(x) C_m^{(\lambda)}(x) C_n^{(\lambda)}(x) (1 - x^2)^{\lambda-1/2} dx = \frac{\pi 2^{1-2\lambda} \Gamma(2\lambda + \frac{1}{2}(l + m + n))}{\Gamma(\lambda)^2 (\frac{1}{2}(l + m + n) + \lambda)} \\ \times \frac{(\lambda)_{(m+n-l)/2} (\lambda)_{(l+n-m)/2} (\lambda)_{(l+m-n)/2}}{(\frac{1}{2}(m + n - l))! (\frac{1}{2}(l + n - m))! (\frac{1}{2}(l + m - n))! (\lambda)_{(l+m+n)/2}}$$

One creative telescoping operator that can be used to prove this identity has the innocent-looking principal part

$$(l + m - n + 1)(l + 2\lambda - m + n - 1)S_m - (l - m + n + 1)(l + 2\lambda + m - n - 1)S_n.$$

We fix the support $\{S_m, S_n\}$ and compare the runtime of the different ansätze. With our implementation of Chyzak's algorithm we need 1122 seconds to get the above, whereas our new approach can do it in 1.6 seconds! Again the reason is that the vector space under the stairs of the Gröbner basis has dimension 8 which is already relatively large and leads to huge intermediate expressions (see Table 1).

3.3. A hypergeometric double sum

The following double sum has been studied by Andrews and Paule [3] from a human and a computer algebra point of view:

$$\sum_i \sum_j \binom{i+j}{i}^2 \binom{4n-2i-2j}{2n-2i} = (2n+1) \binom{2n}{n}^2.$$

This sum being hypergeometric can be treated with both Zeilberger's Multi-WZ implementation in Maple and Wegschaider's MultiSum package in Mathematica (see the footnotes on page 4). We take the latter for a comparison. As already mentioned above, we have to give the correct denominators of the delta parts as input. Then the command `FindRationalCertificate` takes 0.5s to

find the creative telescoping operator

$$1 - (S_i - 1) \cdot \frac{i(2ij - in + i + 2j^2 - 3jn + 2j - 3n)}{(j+1)(i+j-2n)} - \\ (S_j - 1) \cdot \frac{j(2i^2 + 2ij - 3in + 2i - jn + j - 3n)}{(i+1)(i+j-2n)}.$$

Our implementation, having to figure out the denominators on its own, takes a little bit longer, namely 2.1s. We believe that this is still reasonably fast and bet that every user would need more than 1.6 seconds even for only typing the denominators! Using Wegschaider's implementation of the ansatz (2.2) (his favourite method) takes 3.2s and the output is not as nice as the one given above (memory usage: 9MB, output size: 200KB).

We have mentioned that Chyzak's algorithm in principle can be iteratively applied to solve multi-summation problems. This example spectacularly demonstrates that this strategy can end up in a long, stony way: The creative telescoping relations for the inner sum are huge and the tricky boundary conditions make things even more difficult.

3.4. Feynman integrals

Another interesting area of application is the computation of Feynman integrals that is a hot topic in particle physics. We borrow a relatively simple example from the thesis [9, (J.17)]:

$$\int_0^1 \int_0^1 \frac{w^{-1-\varepsilon/2}(1-z)^{\varepsilon/2}z^{-\varepsilon/2}}{(z+w-wz)^{1-\varepsilon}} (1-w^{n+1} - (1-w)^{n+1}) \, dw \, dz.$$

The integrand is not hyperexponential and hence the multivariate Almkvist-Zeilberger algorithm is not applicable (at least not without reformulating the problem). Our implementation needs 174s to find the third-order recurrence in n (but can be reduced to 24s by use of options). Again we can try Chyzak's algorithm iteratively on this example, running into similar troubles as in the previous example, although the swell of the intermediate expressions is by far not as bad as before (note that the input Gröbner basis has only 3 monomials under the stairs). Depending on the order of integration this takes 81s or 171s, but on the cost of higher memory consumption (see Table 1).

4. Conclusion and Outlook

We have described an approach to finding creative telescoping relations that is particularly interesting for multiple sums and integrals as well as for big inputs. For small examples the necessary preprocessing might well consume most of the computation time, but the bigger the input is the less this carries weight. By avoiding the expensive uncoupling step, our ansatz becomes more attractive as the size of the set U (monomials under the stairs) grows. From a theoretical point of view Chyzak's algorithm is still preferable since it is guaranteed to find the smallest creative telescoping relations (with respect to the support of the principal part) whereas our approach involves some heuristics which in unlucky cases can prevent us from getting the minimal output. Therefore we have incorporated several options into our implementation (e.g., for fixing the support of the principal part, the common denominator in the delta part or its numerator degrees) that allow the user to override the built-in heuristics. In the rare cases where this leads to different results, we can compute their union (corresponding to the right gcd in the univariate case) and with high probability end up with the minimal telescoper.

We want to conclude with a really big example to which we plan to apply our method in the near future. In [11] we have presented a computer proof of Stembridge's TSPP theorem using the polynomial ansatz (2.2). The computations for achieving this took several weeks! Attacking the notorious q -TSPP conjecture, which is the q -analogue of Stembridge's theorem, therefore seemed to be hopeless due to the additional indeterminate q that blows up all computations by some orders of

magnitude. With our fast implementation of ansatz (2.3) we can now find the creative telescoping relations for the ordinary TSPP in a few hours! This fact, together with the previous work done in [8] makes it likely that the q -TSPP conjecture can be turned into a theorem after being open for about 25 years.

Addendum to the final version. Meanwhile we have succeeded in proving the long-standing q -TSPP conjecture using exactly the methods described in this paper. The corresponding article has already been submitted for publication [12].

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Christoph Koutschan
Department of Mathematics
Tulane University
New Orleans, LA 70118
e-mail: Koutschan@risc.uni-linz.ac.at